

Article

Simulation of Sustainable Manufacturing Solutions: Tools for Enabling Circular Economy

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Abstract: At the current worrisome rate of global consumption, the linear economy model of producing goods, using them, and then disposing of them with no thought of the environmental, social, or economic consequences, is unsustainable and points to a deeply flawed manufacturing framework. Circular economy (CE) is presented as an alternative framework to address the management of emissions, scarcity of resources, and economic sustainability such that the resources are kept ‘in the loop’. In the context of manufacturing supply chains (SCs), the 6R’s of rethink, refuse, reduce, reuse, repair, and recycle have been proposed in line with the achievement of targeted net-zero emissions. In order to bring that about, the required changes in the framework for assessing the state of manufacturing SCs with regard to sustainability are indispensable. Verifiable and empirical model-based approaches such as modeling and simulation (M&S) techniques find pronounced use in realizing the ideal of CE. The simulation models find extensive use across various aspects of SCs, including analysis of the impacts, and support for optimal re-design and operation. Using the PRISMA framework to sift through published research, as gathered from SCOPUS, this review is based on 202 research papers spanning from 2015 to the present. This review provides an overview of the simulation tools being put to use in the context of sustainability in the manufacturing SCs, such that various aspects and contours of the collected research articles spanning from 2015 to the present, are highlighted. This article focuses on the three major simulation techniques in the literature, namely, Discrete Event Simulation (DES), Agent-Based Simulation (ABS), and System Dynamics (SD). With regards to their application in manufacturing SCs, each modeling technique has its pros and its cons which are evinced in case of data requirement, model magnification, model resolution, and environment interaction, among others. These limitations are remedied through use of hybrids wherein two or more than two modeling techniques are applied for the desired results. The article also indicates various open-source software solutions that are being employed in research and the industry. This article, in essence, has three objectives. First to present to the prospective researchers, the current state of research, the concerns that have been presented in the field of sustainability modeling, and how they have been resolved. Secondly, it serves as a comprehensive bibliography of peer-reviewed research published from 2015–2022 and, finally, indicating the limitations of the techniques with regards to sustainability assessment. The article also indicates the necessity of a new M&S framework and its prerequisites.

Keywords: simulation; modeling; Industry 4.0; supply chain models; DES; agent-based; hybrid simulation; SSCM



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1. Introduction

Circular economy (CE) as a framework presents an alternative to the traditional economy wherein value creation is conceived as being separate and de-linked from the resource utilization [1]. CE, in contrast to the linear economy, bases itself on three principles, namely maximizing the resource utility and efficiency, the extension of the life of the resources and assets, and adding to the lifecycle of the resource or an asset through re-purposing and recycling. In having done so, the CE framework seeks to keep the resources

“in the loop” in a given economy [2]. There is an increased awareness that industrial production and SC activities are one of the principal components of the total carbon emissions. According to a report by the United States Environmental Protection Agency (EPA) they account for 23% of total carbon emissions [3]. As a consequence, there has been an ever-increasing awareness of the need to mitigate the effects of industrialization. This awareness is well reflected in the research community in the recent past which can be gauged from Figure 1. It depicts the prevalence of research with keywords “Manufacturing” AND “Circular economy” and “Simulation” AND “Circular economy” on SCOPUS since 2006. Although there has been an increasing interest in the CE, in the present context, a sustained incongruity between the understanding of CE and its actual realization as social, economical, and, environmental performance in manufacturing-based SCs is greatly lacking [4]. This incongruity can be primarily addressed through use of assessment of sustainability measures that are verifiable, communicable, and widely understood. The use of simulation modeling as a tool for assessing and improving the sustainability performance in manufacturing and SC finds a wide acceptance currently [5]. This can be assessed from the increase in the number of studies in the recent past as shown in Figure 1.

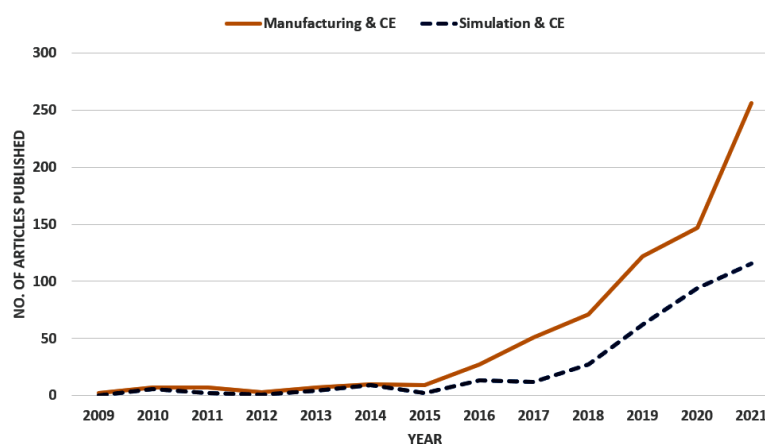


Figure 1. Articles published within CE framework in contexts of manufacturing and simulation. The figure presents the evolution of research in the fields of CE in manufacturing and simulation and CE. The field of sustainability simulation is a fairly new aspect but there has been a steady increase in research in the past few years.

Modeling sustainability in the industrial context covers various aspects of manufacturing and SCs such as in warehousing, logistics, production planning, and resource allocation while invoking various facets of sustainability such as waste elimination, energy efficiency, resource efficiency in manufacturing and SC [6]. The three major simulation tools used to model manufacturing and their allied SCs include Discrete Event Simulation (DES), Agent-Based Simulation (ABS), and System Dynamics (SD). The locales, contexts, and rationale of their application in manufacturing and SCs, although intersecting to a good degree, are diverse and well cut out. These rationales and contexts have in the recent past been expanded into the realm of sustainability analysis. While taking into account their extensive use, they are beset with a number of limitations vis-à-vis the model magnification, data requirements, model validation, and granularity. Doing away with the limitations and anticipating the benefits of combining two or more simulation techniques (such as DES+ABS, ABS+SD, SD+DES, ABS+DES+SD), hybrid techniques find a prominent use in the realm of sustainable manufacturing and SCs. A number of computer-based Modeling and Simulation (M&S) tools are widely available with some of them paid and licensed while others free and open source. This article catalogs some of the free-to-use software in the case of each M&S technique. The literature is rife with numerous techniques that are employed in formulating the simulation models and they are quite diverse unlike the application of

the models themselves. However, a framework wherein these techniques are characterized and brought together with respect to their actual application is severely lacking.

The industry is on the cusp of a new revolution termed as Supply Chain 5.0 (SC 5.0). SC 5.0 seeks to realign the goals of industry from formerly technology-driven growth to value-driven sustainable growth [7]. The SC 5.0 is less of a new technological paradigm and more of an assimilatory philosophy wherein the current technologies are redirected in service of sustainable production and consumption. This includes putting to use the SC 4.0 technologies such as industrial internet of things (IIoT), Cyber-Physical Systems (CPS) and digital twins (DT), augmented reality (AR), and virtual reality (VR) for simulation and modeling of production systems and SCs.

A number of reviews have been published in this framework dealing with various aspects of modeling and sustainability, an exhaustive list of which has been presented in Section 3. Cataloging the simulation methods in sustainability a number of reviews may be indicated, including an article in which the application of three major simulation techniques, namely, Discrete Event Simulation (DES), Agent-Based Simulation (ABS), and System Dynamics (SD) are discussed [8]. Studying various aspects of energy modeling, the studies include a review of software-based simulation tools [9], industrial sector-wise models of energy analysis, energy evaluation and energy-saving following the ISO50001 standard [10], and use of virtual and augmented reality and digital twins for energy modeling [11]. A number of reviews also address the aspect of modeling the product lifecycle [12–15]. The specific contexts where review work has been done includes discrete production environment [16], cyber-physical systems (CPS) [17], knowledge management [18], global and local optimization methods [19], value stream mapping (VSM) [20], and Virtual Reality (VR) [18]. The need for the simulation methodology in manufacturing and their allied SCs, in the present context, is to rise up to the challenge of the long-term global need of manufacturing SCs. The amorphous nature of published research calls for bringing together the diverse themes while taking into consideration a need for a novel framework for M&S. A framework that takes into account the traditional techniques of modeling while incorporating novel technologies such as 3D-printing, Augmented reality, Virtual reality, etc., within the framework of the Circular Economy (CE) paradigm.

Following the PRISMA framework, this article brings together various techniques of M&S and their hybrids finding use in the area of sustainability of manufacturing and SCs. The paper starts with a bibliometric analysis of the collected research works following which a detailed description of the three simulation techniques and their applications is given. A section detailing the various possibilities and resultant characteristics of hybridizing these three techniques is explored. In Section 5, limitations of the current state of the M&S paradigm with regards to modeling CE are discussed and a future course of action is delineated. The paper also includes two appendices. In Appendix A, the exemplary applications of the M&S techniques in the industry in the context of CE are tabulated. In Appendix B, the most commonly used open-source M&S software and their applications in sustainability assessment are tabulated.

In essence, this article

- Indicates the state of published research in the field of modeling of sustainable manufacturing and their allied SCs;
- Assesses the characteristics and circumstances of application of Discrete Event Simulation (DES), Agent-Based Simulation (ABS), System Dynamics (SD), and their hybrids in sustainable manufacturing;
- Underlines the bearings of simulation and modeling on the impending supply chain 5.0 (SC 5.0) paradigm.

2. Methodology and Bibliometrics

This section describes in detail published research in the field of modeling and simulations in manufacturing and SCs within the framework of CE. The bibliometric review approach was created to compare the results of statistically based observational studies

as in medical research, using large datasets; it has since been introduced and is becoming increasingly recognized as a reliable evidence-based review model in management research [21]. This section integrates the systematic literature review with the bibliometric analysis. The PRISMA framework has been followed for selecting the research articles for this review as Figure 2 elucidates the procedure followed for collecting the research articles for this review.

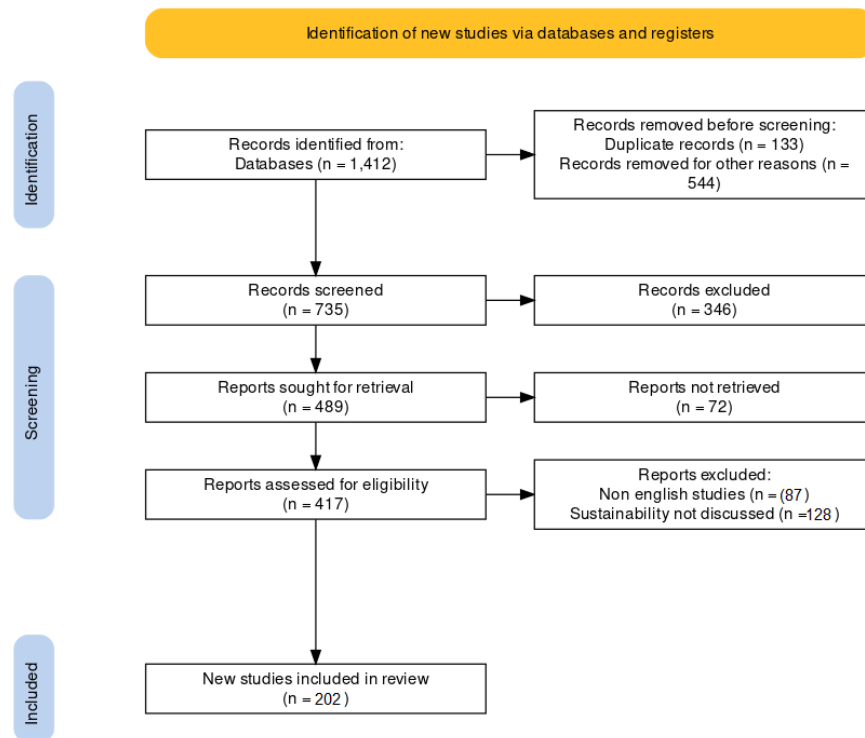


Figure 2. PRISMA flowchart depicting the procedure for collecting the research articles. PRISMA is an evidence-based minimum set of items for reporting in systematic reviews and meta-analyses.

2.1. Selection and Search Strings

The review is composed of the articles composed primarily from the SCOPUS database which is the largest database for peer-reviewed articles and publications. The main elements of the research in question include “sustainability”, “manufacturing”, “simulation”, and “modelling”. The three search strings used are:

1. “simulation” AND “manufacturing” AND “sustainability”;
2. “modelling” AND “manufacturing” AND “sustainability”;
3. “simulation” OR “modelling” AND “supply chains” AND “sustainability”.

On searching of the “Article title”, “Keywords”, and “Abstract” tab in the SCOPUS, the database returned 3559 articles (by April 2022). The search was further limited to “journal articles” with the language in “English” whilst not including conference papers, short surveys, notes, and errata, which reduces the 3559 articles to 1412. Following the PRISMA framework, duplicate records, ineligible papers, and inaccessible records were excluded and 228 papers were retrieved for screening falling in the time frame 2015 to 2022. Adding 74 papers from the other sources, while also including some research preceding the aforementioned time frame, the review is constituted of 202 articles and proceedings. The retrieved papers were put through the Bibliometrix online tool wherein various associations and contours of the collected papers were sought.

2.2. Initial Data Statistics

The 1412 screened articles were published between 2015 and 2022. With the exception of 2022 (142), the number of articles published each year has grown since 2015, as shown in Figure 3. This indicates that academic interest in the given topic is growing.

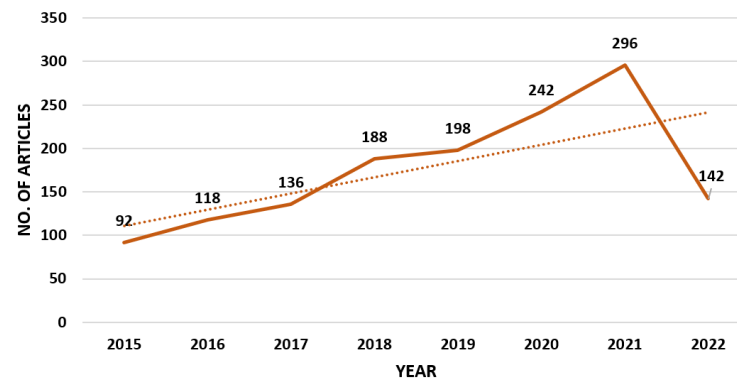


Figure 3. The documents as returned by the SCOPUS database with the above-described parameters and search strings. The number of studies shows a consistent increase as illustrated by the trend line.

2.3. Bibliometric and Content Analysis

Bibliometrics is a statistical analysis of academic publications which includes citation analysis, co-citation analysis, and so forth. In this paper, R-based bibliometrix software using biblioshiny online plug-in is used for bibliometric analysis and preparing the raw data for co-citation analysis. Content analysis is a useful method for systematically reviewing a group of texts. We conducted a content-based literature survey of the 202 articles indicated by the co-citation analysis for six clustering outcomes. We used the deductive strategy to code the articles based on the clustering results of the co-citation analysis, and then used an inductive approach to discover sub-themes inside each cluster by synthesizing the findings of the articles.

2.4. Bibliometric Analysis

The collected papers in this article amount to 202 which fall within the time frame of 2015–2022. The year-wise distribution of the papers included in this review is indicated in Figure 4. As can be gleaned from the figure, the research output on the present theme has remained virtually constant pointing to the continued interest in the topic. Nonetheless, there has been an evolution in the themes that have been taken up in research which are increasingly gravitating towards automation with simulation techniques such as Augmented Reality (AR), Virtual Reality (VR), Digital Twins (DT), and hybrid simulations [22].

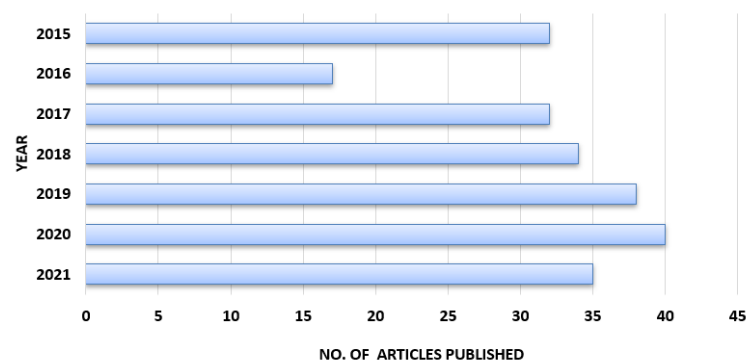


Figure 4. Year-wise distribution of covered research topics. Apart from the papers spanning the time frame 2015–2021, which form the mainstay of the research, some of the papers which provide supportive evidence to the research results have not been cataloged above.

The research results collected for this review spans the globe and have been published in various journals. The topical relationship between the countries, keywords, and the publishing journals is depicted as three-field plot in Figure 5. The three-field plot in large part agrees with the country citation index such that India, USA, Italy, and Germany have 30, 31, 16, and 14 articles, respectively. Besides this, the sources which have been published most on the present topic include the journal of sustainability (Switzerland), Procedia CIRP, and Journal of cleaner production with 15, 12, and 14 articles respectively included in this review. The keywords that mediate between the two in the plot are typical of the research theme and include Supply chain 4.0, energy efficiency, and simulation, etc.

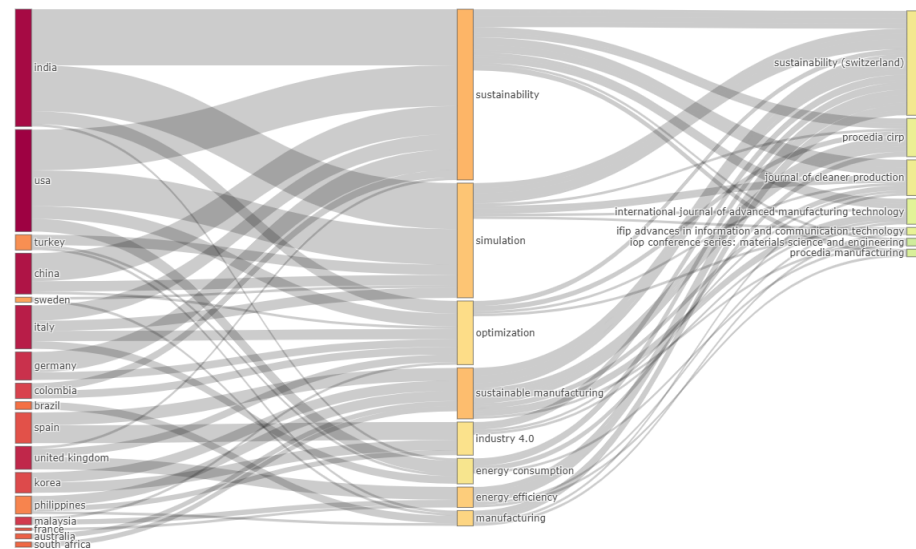


Figure 5. The three-field plot or the Sankey diagram showing the relationship between the publishing countries, author keywords, and the journals. The figure shows the most significant studies in the present context which appear in peer-reviewed journals. India, USA, and Turkey being the most significant publishing countries with sustainability (Switzerland), procedia cirp, and journal of cleaner production being the most significant journals.

The abstracts of the collected papers were analyzed, using the Bibliometrix application, for the recurrent themes and words. Excluding the trivial words and focusing on two-worded and three-worded themes, a thematic tree map was generated which is shown in Figure 6. The theme of energy simulation and modeling dominates as it is also reflected in the amount of research dedicated to this topic. A total of 40 papers in the collected research area directly or indirectly deal with this topic. Some of the most-cited of those papers include themes such as simulating energy conservation in the milling process [23,24] and selective laser melting [25], etc. Besides this, lifecycle assessment shows a frequent presence in the abstracts. Some of the research includes topics such as social LCA [13], system dynamics and LCA [26], lifecycle cost assessment, and LCA [27], energy assessment and LCA in the Industry 4.0 [28], sustainable machining process [29], and lifecycle inventory gate-to-gate process energy use [30], among others. An alternate theme of the product lifecycle is also present in the abstracts which is similar to that of the LCA. A contemporaneously important topic of additive manufacturing also finds use in LCA [31–33].

The collected literature was subjected to the Bibliometrix online tool wherein, using the co-occurrence analysis on the 492 keywords, a keyword network was generated. The keyword network, showing the outline of published research, is depicted in Figure 7. The four clusters are named according to characteristic keywords. They are the lifecycle assessment cluster, decision support system, manufacturing methods, and numerical model. The cluster of product lifecycle includes themes such as environmental impact, benchmark, energy efficiency, and costs [10,34–37]. The cluster of decision support system includes

themes such as economics, operations, planning, investments and competitions addresses topics such as enterprise resource planning through simulation [38], real time control [39], energy investment [40], green investment [41], and agent-based simulation for scheduling in a competitive environment [42]. The third cluster termed energy modelling methods includes themes such as machining, resource efficiencies, and cutting tools including topics such as energy consumption in machining [24,43,44], manufacturing systems using a digraph-based approach [45], and sustainable CNC milling [46]. Finally, the fourth cluster termed numerical model includes topics such as product mix for the process industry [47] and NSGA-II algorithm for the process planning problem [48].

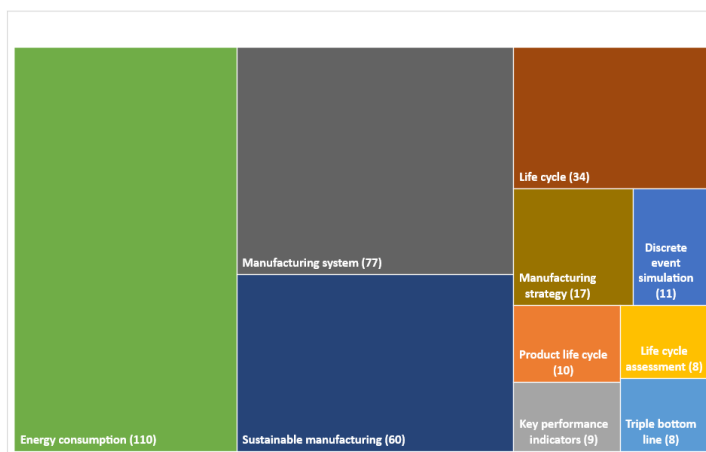


Figure 6. Tree map of the keywords mined from the collected abstracts. The keywords were mined from the abstracts of the collected research articles. The single-worded keywords were excluded from the map and only the two-worded and three-worded keywords were selected in the research articles to better reflect the contours of the collected research theme.

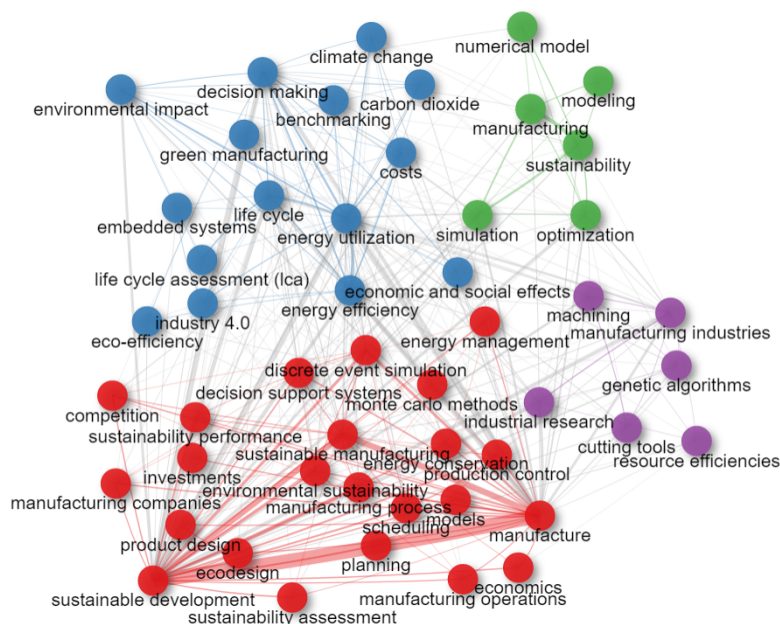


Figure 7. Keyword network of the published research works. The keyword network shows four prominent clusters of co-occurrences. The counting of matched data inside a collection unit is known as co-occurrence analysis.

3. Meta-Review of Reviews

Several reviews published recently have attempted to approach the topic at hand differently. Since the motivations of this review are broad-ranging, the possible topics that

this review seeks to incorporate are many. An exhaustive list of these reviews is tabulated in Table 1.

Table 1. Recently published literature reviews with thematic proximity to this article. The articles span various topics, including simulation tools such as LCA and sustainability assessment, among others.

Author	Title	Year
de Mello Santos V.H., Campos T.L.R., Espuny M., de Oliveira O.J. [49]	Towards a green industry through cleaner production development	2022
Mies A., Gold S. [50]	Mapping the social dimension of the circular economy	2021
Birkel H., Müller J.M. [51]	Potentials of industry 4.0 for supply chain management within the triple bottom line of sustainability—A systematic literature review	2021
Anaruma J.F.P., Oliveira J.H.C., Anaruma Filho F., Freitas W.R.S., Teixeira A.A. [52]	The first two decades of Circular Economy in the 21st century: a bibliographic review	2021
Yasamin Eslami and Mario Lezoche and Hervé Panetto and Michele Dassisti [53]	On analysing sustainability assessment in manufacturing organisations: a survey	2021
Machado M.C., Vivaldini M., de Oliveira O.J. [54]	Production and supply-chain as the basis for SMEs’ environmental management development: A systematic literature review	2020
Furstenau L.B., Sott M.K., Kipper L.M., MacHado E.L., Lopez-Robles J.R., Dohan M.S., Cobo M.J., Zahid A., Abbasi Q.H., Imran M.A. [55]	Link between Sustainability and Industry 4.0: Trends, Challenges and New Perspectives	2020
Micolier A., Loubet P., Taillandier F., Sonnemann G. [56]	To what extent can agent-based modelling enhance a life cycle assessment? Answers based on a literature review	2019
Sassanelli C., Rosa P., Rocca R., Terzi S. [57]	Circular economy performance assessment methods: A systematic literature review	2019
Ahmad S., Wong K.Y. [58]	Sustainability assessment in the manufacturing industry: a review of recent studies	2018
Garwood T.L., Hughes B.R., Oates M.R., O’Connor D., Hughes R. [9]	A review of energy simulation tools for the manufacturing sector	2018
Moon Y.B. [8]	Simulation modelling for sustainability: a review of the literature	2017

Figure 8, a keyword network of the recently published reviews, promptly exhibits the breadth and diversity of the topics that these reviews address. Among those topics belongs the topic of sustainability indicators or sustainability KPIs. This theme has been approached by a number of reviews. Indicating the 144 sustainability metrics along the three aspects used in manufacturing, a review [59] undertook the maturity analysis of the (key performance indicators) KPIs. It concluded that there is an inconsistent usage in KPIs, particularly in social and economic aspects. Another review along the same lines adopted the division of “sustainable manufacturing” and “manufacturing sustainable” while also incorporating account facility design and supply chains into manufacturing within the “6R” framework. Discerning the need for appropriating social sustainability indicators in manufacturing, a number of reviews have been published recently. Covering five aspects of social sustainability, namely organization, workers, customers, local community and society at large within the circular economy framework, the review [50], while seeking to clarify the concept, characterized the indicators along three perspectives, namely, micro, meso, and macro levels. Another review [60] focusing on social sustainability, on basis of the collected research works, concluded that creating job opportunities is by far the most important of the indicators while pointing to the need for aggregation approaches. One may also indicate the reviews investigating social performance as an aspect of organizational performance [61]. The social aspect of CE has also been understood through lifecycle assessment termed as the social lifecycle.

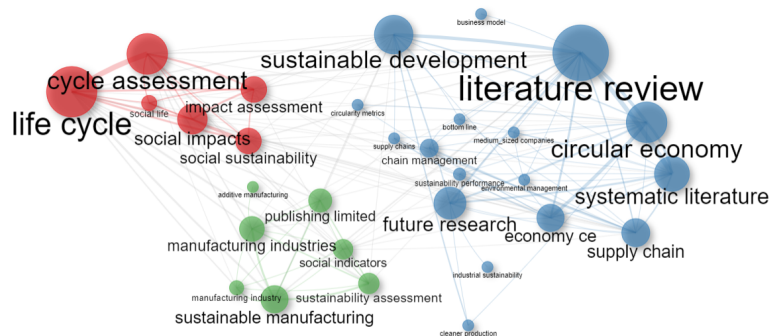


Figure 8. A keyword network of the published reviews in the field. Besides showing the pre-eminence of the CE and lifecycle assessment, the keyword network also presents sustainability-related concepts that deal with the idea whole paradigm of manufacturing rather than just the actual process of manufacturing.

A review [14] concluded that the guidelines for operationalization, application, and measuring of social indicators as being limited leading to bottlenecks in gathering data and identifying stakeholders concerns. Another review charted out the history of social lifecycle assessment, dividing it into four stages wherein the present era is termed as that of the standardization [15]. Another aspect that this seeks to incorporate is that of simulation, modeling and optimization within the CE framework. A number of simulation techniques have been researched into and they include pinch analysis, P-graphs, and AI/ANP (Artificial intelligence/Analytic Network Process) [62], review of energy simulation tools [9], review of ABS, DES and SDM simulation techniques [8], and a review of agent-based simulation with LCA techniques [56].

4. Simulation Models and Sustainability: Characterization

This section shall provide an exhaustive overview of the simulation models in use in the context of sustainability in SC. Simulation models can be characterized along three fundamental aspects:

- Assessing the temporal aspect of the processes;
- Taking into consideration the randomness of the processes;
- In view of the organization of the process data.

If the factor of time is addressed in the simulation, it is called a dynamic simulation and if not, it is termed as a static simulation. Dynamic modeling emulates an existing or possibly feasible system state to analyze the dynamic relationship between model variables and, in the case of sustainability, it generally consists of resorting to the use of the systems approach [63]. Dynamic simulation can further be classified as continuous or discrete such that in discrete simulations, the changes do not occur continuously but at given times. In the continuous simulation, the changes are assumed to have occurred continuously. Discrete event simulation is further characterized as time-stepped simulations and event-driven simulations. In the former, time intervals are assumed to be equal whereas, in the latter, the events or changes in the system are marked rendering the time intervals as unequal.

A number of studies have compared continuous simulation and discrete event simulation. Sustainable manufacturing processes have been modeled and compared using both discrete event and system dynamics simulation so as to ascertain aspects that are appropriate for each modeling approach [64].

On the other hand, based on randomness, the simulation may be described as being deterministic or stochastic. In a deterministic simulation, each simulation run gives the same result whereas it is not the same in the case of the stochastic simulations. A study comparing the sustainable production planning approaches using deterministic and the stochastic method may be cited. A decision framework is presented which may guide the managers to choose between the two [65]. Finally, with regards to data management, a

simulation can be either a grid-based simulation or a mesh-free simulation. A grid-based simulation construes a manufacturing plan as discrete cells and the simulations are done such that the relationship between various cells is taken to account. A mesh-free simulation derives data while conceiving individual entities [66]. The literature deliberates upon the issue of model resolution. Multi-resolution modeling is presented in contrast to hierarchical modeling [67]. In the case of modeling sustainability in manufacturing and SCs, the idea of multi-resolution modeling is presented as fundamentally essential as simulating sustainability in any context includes dealing with different levels simultaneously. Multi-resolution modeling is defined as the approach whereby a complete model is approached or parts of the model with different resolutions are addressed. It is brought about in a way whereby long-term questions are solved with low resolution whereas short-term questions use higher resolution models. An improvisation on the concept of multi-resolution modeling is the idea of a sustainable cockpit [68]. Additionally, the model presents a continuous modeling technique all the while conceiving of the system in discrete terms. Another aspect of the simulation is what is termed model magnification. Model magnification has been alluded to in the literature along different time frames. Models have been defined as being strategic, tactical, and operational [69]. Strategic models refer to time frame from five to ten years. Tactical models are addressed to time frames from few months to two years, and the operational modeling deals with the weekly, daily or hourly operations. In context of manufacturing and supply chains, the strategic modeling spans the organizational design, facility location, product development, supplier selection, etc. The tactical modeling includes problems such as warehousing, maintenance, and stowage handling. Operational modeling deals with scheduling, lot size assessment, and workforce planning, among others.

In manufacturing, various simulation tools have been employed with the majority of the research works and applications using the following simulation tools:

- Discrete Event Simulation (DES);
- Agent-Based Simulation (ABS);
- Systems Dynamic models (SD);
- Hybrid models.

Figure 9 indicates the growth of research in DES, ABS and SD simulation models in manufacturing and SCs as gleaned from the data from 2000–2021 on the SCOPUS database. The DES found great use early on, while SD and ABS are slowly catching up.

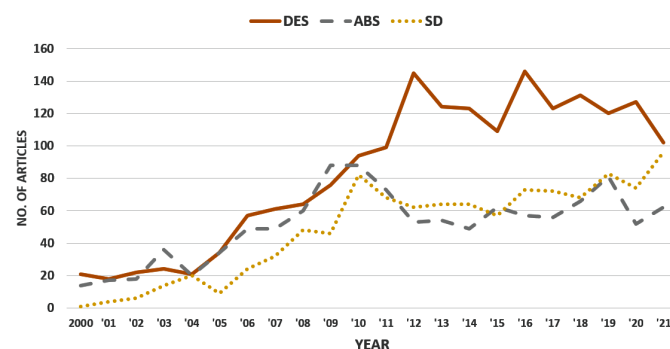


Figure 9. Yearly research output across the three simulation techniques. The figure shows the research output in case of the three simulation techniques in the field of manufacturing and supply chains as gathered from the SCOPUS database. Although DES far outnumbers the other two initially, there has been increasing research in SD.

As can be gleaned from Figure 9, DES is the most used simulation method in the published research works [70]. Comparing the DES with the SD, the DES is applied in the cases where queuing of some sort is being used, whereas SD is used in the systems which are dynamic and thus exhibit a “flow”. The DES thus deals with the microscopic level such that they take into account the smaller details of the system. The consequence

of this is that there is a greater requirement of data in the case of DES and it should be of high quality [71]. Furthermore, when the DES is applied in the case of a production system, there is a requirement that there is a constant updating of the data as well [72]. SD employs a system framework while using flows, stocks, and feedback loops to model the behavior of the system through time [73]. The SD, on the contrary, has a macroscopic perspective and takes into account a wider perspective. SD and DES also deal differently with randomness. DES is stochastic and, therefore, for each given run gives a different result, whereas the SD is deterministic and gives the same results for each run. The process of model building has been compared in the case of SD and DES [74]. The modeling in DES on average takes more time than the SD and, therefore, it is assumed that DES is more complex than the SD modeling. DES allows investigators to model the progression of a given system, e.g., the advancement of a product through an assembly line—and is frequently used to depict a system’s business operations. When the temporal fluctuation of the states of system elements is an important source of variability in the system’s outputs, this technique is particularly well suited. Although SD and DES may generate identical findings, the method used may have an impact on the system’s limits and how an investigator addresses a given issue [75].

Other comparisons cited in the literature [76] are:

- Animations are fundamental to DES whereas model descriptions are more important to SDs;
- SD models are more representative of the problems than DES models;
- SD aids in conceptual learning more than DES;
- Results of DES are more difficult to interpret than that of SD.

Recently, a good deal of research has been conducted by taking up the hybrid approach wherein both SD and DES are used together. Some of the instances in case of manufacturing include use cases, including performance analysis [77], re-configurable manufacturing [78], value chain environment [79], etc.

ABS, unlike the SD and DES, is a context-dependent modeling technique and unlike the top-down approach as used in SD, it uses a bottom-up approach in modeling such that the behavior of the whole system is determined by the interaction between the agents [73]. Although the ABS unlike SD is stochastic but according to Agency Theorem for System Dynamics, SD models are basically subsets of ABS models [80]. This implies that all the SD models can be modeled as ABS models but that comes at a greater cost as ABS models are complex and time-consuming. Like DES, ABS has stochastic nature and models random behavior but there are major differences. In the ABS, in contrast to the DES, the agents are modeled with behavior and thus are termed as active. Additionally, the ABS does not use queuing like DES although, in some hybrid DES models, some entities may be modeled as active. Figure 10 depicts the comparative applicability of the simulation models with respect to their abstraction level and magnification.

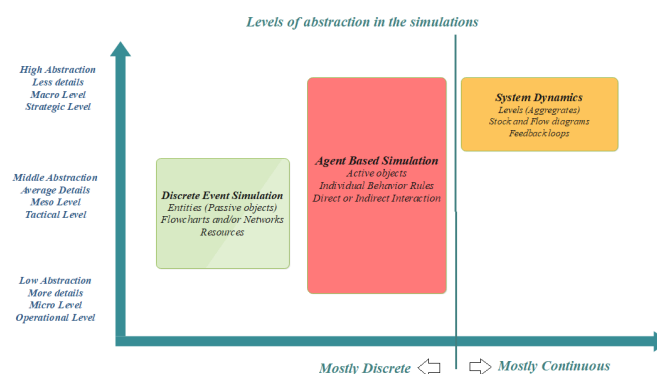


Figure 10. The figure shows the levels of abstraction that the three simulation techniques are capable of. The amount of data required for a model is inversely proportional to its level of abstraction.

4.1. Discrete Event Simulation (DES)

Discrete event simulation originally appeared in the late 1950s, and it has slowly increased in popularity to become the most widely utilized of the traditional operational research methodologies across a wide range of industries, including manufacturing, travel, banking, health, and beyond. A discrete event system (DES) is a discrete-state and event-driven system in which the state changes only as a result of discrete events occurring across time. Event-based modeling refers to the representation of the information of the discrete event system using an event graph. The representation of temporal and logical relationships between the event is called an event graph [81]. An event graph consists of a set of event nodes and directed edges with two types of edges described as scheduling edges and canceling edges. An event-based model allows the system to evolve through a sequence of events such that an event is described as a change in the state of the model. A discrete event modeling is defined, in contrast to continuous modeling, as the system that changes discretely at certain points in time [82]. As the events taking place in the system are random, therefore, any description of the system using differential equations is not possible; thus, the requirement of the event graphs is warranted. The components of DES include the following items

- System State: The collection state variables which, at a given time, describe the state of system;
- Simulation clock: It describes the current time in the system;
- Event list: List made up of list of events taking place at a given time in the system;
- Statistical counters: Variables that have statistical system data stored in them;
- Initialization routine: An algorithm whereby the simulation is initialized at time zero;
- Timing routine: An algorithm that draws up sequence of events with time;
- Event routine: Algorithm that updates the system state after an event has occurred;
- Library routines: Random observation generator from probability distributions;
- Report generator: Algorithm that estimates the optimal measures and stores them as reports;
- Main program: This is an algorithm that, using the timing routine, determines the next event and thence shifts the control to the event sequence and updates the system.

The magnified and data-dependent view of DES implies that its application in manufacturing SCs is generally limited to the operational level. Nonetheless, some instances where DES finds its use at strategic-tactical level of operations include: design of new facilities [83], improvement of warehouses and distribution centers [84,85], changes in staffing and operating rules, and effect of investments on facility operation [86,87], among others. DES has historically been invoked in the case of sustainability through the lens of optimisation such that sustainability was conceived as a sub-problem of optimization. The earlier approaches to sustainability using DES were limited as “optimization of multiple objectives was not very common in manufacturing simulation” [88]. The evolution of DES software rendered them useful in the case of complex systems such as logistics, healthcare, military strategy, and profit optimization. One of the major issues applying DES for sustainability can be attributed to limited computing power in the past. The limited size of memory limited the size of the models that could have been developed. The clock speed also limited the simulations that could be run. However, in the recent past, there has been a steep increase in the computing power available to researchers and practitioners. Following this, a number of studies appeared where DES was applied in the case of sustainability assessment. The use of DES for modeling sustainable operations in manufacturing SCs has been carried along two major themes. Firstly, those problems that deal with the material flow in industrial and their allied operations and, secondly, those dealing with energy flows in the operations. The reason for this is that DES requires extensive data which are objective and translatable into numbers. This is easily achieved in case of energy modeling and flow modeling where data are easily available. The focus of DES on the operational modeling of sustainability is well exemplified by a study where material and energy flows are modeled in an industrial setting using DES. The model has been applied by decom-

posing the factory into infrastructure, process chains, individual processes, and building service systems. The energy and material flows are modeled using machine utilization and energy demands over time. The dynamic inter-dependencies were also taken into consideration [68]. Another recent instance of the application of DES with operational concerns is a study wherein sustainable manufacturing is conceived as being a function of energy management [89]. The study uses real-time online DES to model renewable energy sources with the intention of reducing carbon dioxide emissions and energy costs. The study uses ERIM-P (Energy Resources Intelligent Management-Predictor) data prediction in combination with ERIM-RT real-time data of manufacturing plant and weather conditions. Nonetheless, DES also finds use at the policy-strategic level. A specimen of this is a study that models the product lifecycle using DES. Termed lifecycle simulation, the DES is used to simulate the material flows [90]. The calculation is carried out using DES wherein the total amount of pollutants, waste, energy usage, costs, and profit of the company for a given period are considered. In order to better understand the application of DES for assessing sustainability, various aspects of DES models have been lined up with their efficacy with regards to sustainability assessment in Table 2. As can be discerned, the DES with regards to sustainability is beset with two major limitations. Firstly, DES is limited by scope and abstraction level and, secondly, DES requires large and precise datasets to model a system. Another issue with DES is that, with the increase in the complexity of the modelled system, its complexity increases exponentially; as a consequence, the use of DES has been limited to operational-tactical levels. In case of the first limitation, the issue has been alleviated using hierarchical modeling. The higher levels are modeled using SD or ABS while DES is used for micro/operational levels. The data dependency of DES has also been addressed using ABS and SD [91].

A detailed description of simulation hybrids is presented at the end of this section.

Table 2. Major aspects of DES and their efficacy with regards to modeling sustainability.

Criteria	DES	Effects on Sustainability Assessment
Approach	Process-based	Process-centered sustainability assessment eschews the organizational/systemic view focusing on a given process, e.g., resource flows [92]
Object	Entity	Objects in a system are distinct individuals. Limited behavior with the environment, thus does not exhibit emergent behaviors, thus limiting the use in socio-economical contexts. It also cannot capture proactive human centric behavior. Limited ability to adapt the structure at runtime [93].
Space/Time	Discrete	Sequential process models. State changes occur at discrete points of time. Models are simulated in unequal time steps, when ‘something happens’ [94].
Feedback	Implicit	Feedback, delays and nonlinearities are not emphasized which in case of sustainability assessment renders strategies as static
Randomness	Stochastic	Randomness explicitly modeled with the appropriate statistical analysis, complexity increases exponentially based on the size and requirement [94].
Predictive power	High	High predictive power whereby actual flows are determined, e.g., carbon dioxide emission assessment [95]. The human agents are well-defined decision makers as the output takes form of point predictions.
Abstraction level	Meso-Micro	Sustainability assessment at lower individualized functions, e.g., solid waste management [96]
Scope	Operational-Tactical	The sustainability assessment for short time range, e.g., integrating human factors in manufacturing with simulation runs of one month [97]
Data	Quantitative	Data to be sourced from plant databases which includes energy utilization, emissions, resource utilization, etc. Data from a CNC for energy utilization as an example [98].
Use-case	Optimization, Prediction and bottleneck analysis	Sustainability is conceived within the rubric of optimization. Energy optimization cases are the most common examples [99].

There are 27 articles that deal with simulating sustainability using DES in the industrial context. Some of the studies use DES singly while others make use of the fusion of one or more simulation techniques in addition to DES. Appendix A.1 indicates the recent representative research wherein DES has been used in modeling sustainability in manufacturing and allied SCs. Models using more than one simulation technique are termed hybrid models. The collected articles on DES and sustainability include both pure and hybrid models and can better be characterized by the keyword network of those papers. The keyword network as shown in Figure 11 indicates the thematic constitution of those articles. Most of the articles focused on the operational level with the theme of energy modeling or simulation dominating the aspect taken up by the researchers. In addition to the ones pointed out to in Table A1, one may indicate other studies in contexts including the digital factory concept [100], input data management [101], and water-energy nexus [102], among others. The pre-eminence of energy modeling again points to the fact that DES requires extensive and precise data which are easily available in case of energy use in manufacturing and SCs. Other aspects of sustainability, such as social factors, which show up at higher levels of abstraction do not show up as often in the context of DES.

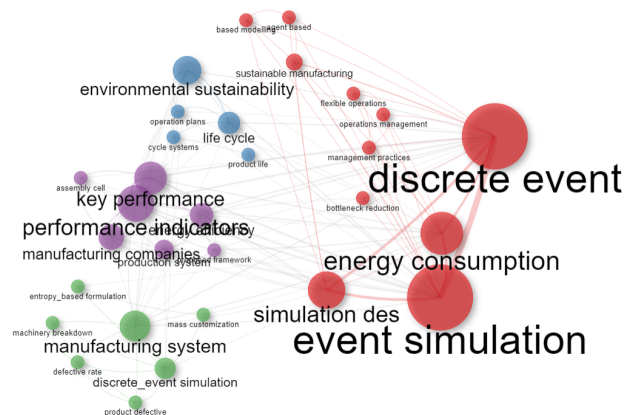


Figure 11. The figure shows the network of keywords used in the collected papers where DES is utilized in sustainability assessment in the case of manufacturing and SC. The network shows a pre-eminence in energy consumption and management. Bottleneck reduction and assembly cell also find a dominant place in research pointing to DES being predominantly used at the operational level.

The aspect of sustainability in manufacturing and SC has been studied along various aspects of industrial production in the recent past using DES. Table A1 indicates various case-based studies on different aspects of sustainability that have been undertaken in manufacturing and SCs using DES.

The use of software in case of DES has its beginnings in early 1960s when software such as SIMULA, GPSS, and SIMSCRIPT were developed. In the 1970s and 1980s, SLAM, GPSS-H, VIS, WITNESS, HOCUS, GENETIK, SIMAN/CINEMA, and ProModel arrived on the scene. Most of these software were expensive each costing in excess of 1000 \$. With increasing computing power, some low-cost software solutions were introduced in the 1990s. Some of the examples included Simul8, Extend, and ShowFlow. In recent times, a large number of DES tools have been conceived and are in use. Most popular tools in DES include Anylogic, Arena, ExtendSim, PlantSimulation, Simul8, SimEvents, VisualSim, and Witness. However, owing to high license fees, these tools are generally out of the budget of researchers. Table A4 indicates some of the well-known open-source tools in the DES.

4.2. Agent-Based Simulation

Agent-based Simulation/Modeling (ABS/M) or Individual-based modeling (IBM) has been developed as a solution to the need for modeling natural systems [103]. It finds its conceptual beginnings with the examination of complex systems, adaptive systems, and modeling of biological systems. The ABS constructs a conceptual model through a

bottom-up approach, by taking into account discrete entities or agents with an assumed behavior which is then simulated using software [104]. “Agent” is a representation of a component that is present in a “social” setting and that may or may not be construed as being intelligent [105]. The agents are presumed to be both individuals as well as collections (such as groups, networks, etc.). A benefit of using agents in the case of simulation is that they address both autonomy and complexity as they are distributed, adaptive to changes, and exhibit intelligence. They may also show learning behavior and rationality while using simple decision-making rules [106]. The characteristics of the agents are described as:

- Agent is located in a dynamic environment and behaves autonomously and intelligently in that environment;
- The environment of the agents can have other agents and the system, as a consequence, is known as multi-agent system.

Consequently, the agent-based models are composed of the following:

- Various agents with specified agent granularity;
- Rules for making decisions;
- Learning rules whereby the agents modify their behavior based on past outcomes;
- Social interaction of the agents;
- The environment.

As described below, Figure 12 depicts the structure of a typical agent-based model.

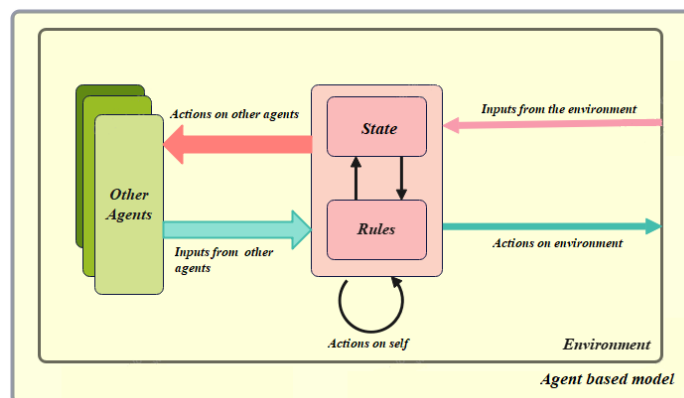


Figure 12. The figure describes how an ABM is built from the bottom. The autonomous and interactive nature of the agents renders complex modeling possible. The agents in addition to interacting with other agents can also interact with the real-world actors as well.

Some of the advantages of using agent-based models cited in the literature include [107]:

- Agents are individually modeled and consequently monitored which makes determining the state of the agent at a particular time easy;
- Possibility of modeling large-scale complex systems which are also termed massively multi-agent systems (MMAS);
- ABS while capturing the emergent phenomena. The emergent phenomena may have characteristics different from that of the constituents of the system that ABS is able to capture. Many agent-based models exhibit the trait of emergence, which happens when some attribute that may be expressed at the system level is not expressly encoded at the individual level;
- ABS provides a natural description of the system while retaining flexibility. The property of natural description in ABS is linked to the presence of behavioral characteristics of the agents. Whereas flexibility refers to the possibility of adding or subtracting the agents from the model when needed.

The application of the ABS has benefits over other simulation techniques. However, owing to high costs and complexity, these benefits are not absolute. The ABM is computationally intensive as simulation a large number of agents requires huge computational

power. ABM also requires that the modeler should have data regarding the elements of the model, as without any knowledge or an educated opinion of the operation of the system, it is not possible to build the model.

In recent times, the use of ABS has been at the forefront in research and has been applied more than DES and SD. Appendix A.2 indicates the recent representative research wherein ABS has been used in modeling sustainability in manufacturing and allied SCs. The reasons for this are that there is greater propagation, availability of software, and education. The reasons cited for this have been a positive feedback [8].

The use of ABS in case of sustainability has been proposed in place of tools such as lifecycle assessment (LCA), Strategic environment assessment (SEA), Environmental impact assessment (EIA), and multi-criteria analysis (MCA), among others [108]. ABM is increasingly being used to investigate the formation of complex nonlinear phenomena in connected human and natural systems [109]. With the ABM, various agents, including organizations, agencies, and actors can be modeled, while also simulating the environment containing them. The ABM, unlike other methods, can simulate heterogeneity which finds greater use in contexts where individual decision-making with diverse objectives is taken into account in addition to the changing social, economical, and environmental behaviors [110]. Modeling sustainability with ABS has shown to be a promising strategy. It is claimed that detecting macro-behaviors aids in the comprehension of complicated physical and ecological systems [111]. The primary idea of an ABS model is to describe interactions between social-economic and ecological processes. Along the general environmental theme, the ABS has found a great deal of application. The ABM provides for flexibility in modeling such that it may be as sophisticated as the computing power allows for. Such that when it comes to sustainability, the ABM can also be integrated with other frameworks including the LCA. The degree of integration is assessed by the expected outcome. Research also shows that the use of ABM enhances studies where limited computational power is available [112]. Those models which were formerly developed using econometric methods and nonlinear programming techniques were enhanced using the ABM [113]. Furthermore, ABM also allows for incorporating human behaviors. The case of modeling human behavior in the case of sustainable logistic management may be cited [114]. Sustainability has been addressed using ABM in research along one of the four categories. The first category includes studies modeling traditional issues of pollution control [115]. The second category deals with resource modeling such as energy, oil, land, etc. [116]. The third category involves studies that deal with diffusion of sustainable behavior which also include market and policy-based models [117,118]. The fourth category includes modeling global environmental issues. Examples of which include [119,120]. This study has included research covering the first and second categories. SCs can be conceived as consisting of supply (procurement logistics), production (manufacturing systems), distribution (delivery), and reverse logistics (planning and implementation) [121]. In case of manufacturing SCs, ABS has been put to use across all the four areas, instances of which include waste paper [122], manufacturing resource efficiency [123], carbon-based freight consolidation [124], and SC planning [125]. With regards to magnification, ABS finds use at all three levels of operation. A study encompassing the strategic level seeks to model sustainable industrial policy using by coupling macro-economic dimensions with environmental parameters while optimizing the resource efficiency [123]. The application of ABS at the tactical level is exemplified in a study where industrial collaboration is modeled wherein a space of cooperation between industrial partners is explored in an economically win-win manner [126]. At the operational level, the ABS in optimizing the real-time energy consumption of resources in job-shop manufacturing processes. The data used for simulation are collected from industrial robots [127]. To understand the application of ABS for assessing sustainability, various aspects of ABS models have been lined up with their efficacy with regards to sustainability assessment in Table 3. Since sustainability models engender high complexity, ABS models often take a long time; therefore, they cannot give the “quick and dirty” solutions that simulation is frequently employed to find [74]. In such cases, DES has been

used as a hybrid that outperforms the ABS in performance. Among the articles collected for this review, 21 deal with ABS in manufacturing and SC in the sustainability framework exclusively, whereas in 12 articles, ABS is used as a tool hybridized with other tools. The keyword network of these papers is shown in the Figure 13. The keyword network shows five clusters.

Table 3. Major aspects of ABS and their efficacy with regards to modeling sustainability.

Criteria	ABS	Effects on Sustainability Assessment
Approach	Bottom-Up	Action of agents result in population wise changes making possible sustainable emergent behaviors, e.g., sustainable supplier populations [128]
Object	Agent	The environmentally aware agents make possible human thinking and model for social processes [129]. ABM consolidates irrational choices driven by socio-economic and cultural components.
Feedback	Implicit	Integrate the awareness of the environmental impact of agents choice to their decision-making process. Incorporated in number of sustainability studies, e.g., in coupling between LCA and ABS [56].
Space/Time	Discrete/Continuous	ABM used to explore spatial and temporal dynamics for environmental awareness. Market dynamics to assess green product design impacts [56]
Predictive power	Highest	Agent behavior prediction is highest among the three in ABS. Sustainability assessment may further augmented with ML algorithms, big data, and neural networks, e.g., green SC [130], sustainable intelligent manufacturing [131].
Abstraction level	Micro-Meso-Macro	ABS is capable of modeling sustainability at all the three levels from the shop floor to national carbon trade, e.g., carbon trade [132], sustainable industrial symbiosis [133], and closed loop production planning [42]
Scope	Operational-Tactical-Strategic	Due to its functioning at both detailed level and aggregated level is used at all the three levels, while incorporating both qualitative and quantitative, ABS exhibits multi-granularity. Resource sharing [134], industrial symbiosis [133], and investment efficiency [123] constitute the three temporal levels.
Data	Quantitative & Qualitative	The data magnification in ABS is highest among the three, incorporating both costly factory floor measurements and delphi-style information.
Use-case	Emergent phenomena, adaptive situations, proactive, and reactive behaviors	Owing to greater computing power ABS is used to model to high accuracy sustainability transitions, e.g., socio-technical transitions [135]

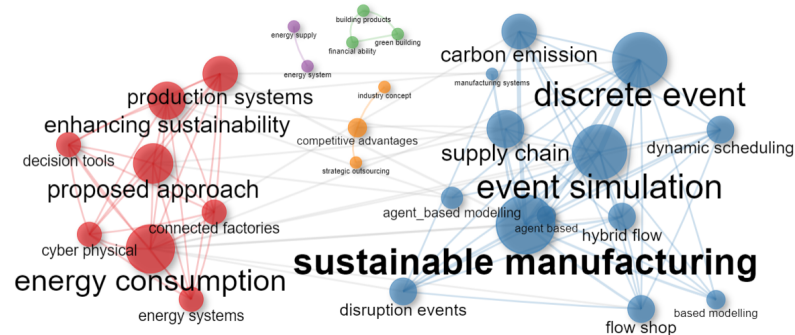


Figure 13. The figure shows the network of keywords used in the collected papers where ABS is utilized in sustainability assessment in case of manufacturing and SC. The network show a pre-eminence of “sustainable manufacturing” and “energy consumption”. The prevalence of “discrete event simulation” points to frequency of the two simulation techniques being hybridized together.

The agent-based models have been realized using both domain-specific and general-purpose languages. Some of the domain-specific software includes spreadsheet programming tools, Mathematica, and agent-based languages such as Anylogic, MATsim, Repast,

MASON, NetLogo, and Swarm. In addition to these, numerous open-source and free software is available as well—a detailed list with their application is indicated in Table A5.

4.3. System Dynamics (SD)

SD is a top-down modeling framework, originally proposed in 1961, with information feedback aspects. An SD model is used to investigate a dynamic evolution process in various scenarios. Reductionism and holism, as philosophical paradigms, have been cited as the basis for SD modeling. Reductionism, through simplifying ideas, is the act of reducing complicated structures, concepts, or events into their constituent parts. Alternatively, SD is also said to be holistic in its approach to understanding a system's dynamic behavior in comparison to existing issue description and solution methodologies [136]. Causal Loop Diagrams (CLD) maps the feedback loops showing the dynamic interactions of the system variables. The variables are connected using arrows that depict causal relations between them with the indication of positive and negative polarities [137]. The polarities signify the nature of the relationship between the variables as they specify how the dependent variable influences the independent variables. The feedback loops are characterized as balancing and reinforcing. Positive feedback indicates that a change in any of the variables in the causal loop will eventually have a positive effect on itself, whereas negative feedback indicates that a change in any of the variables in the causal loop will have a negative effect on itself. In its methodology, the SD has four major stages, namely, the conceptual stage, causal loop stage, simulation stage, and model evaluation. These stages are depicted in the flowchart in Figure 14.

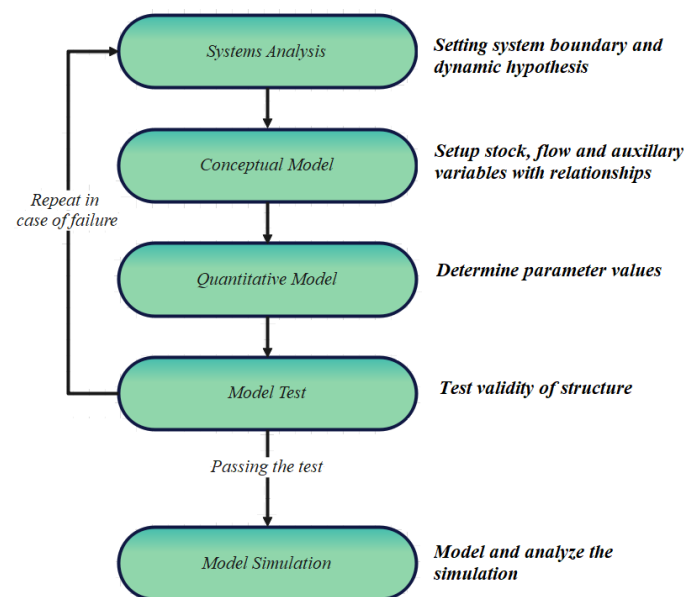


Figure 14. The model creation and simulation process is depicted in a flowchart. The system analysis stage, the establishment of the conceptual model stage, the construction of the quantitative model stage, the model verification stage, and the model simulation stage are all covered by the fundamental technique of SD modeling.

Among the three simulation techniques, the SD is considered as being most commensurate with the breadth of analysis that sustainability modeling requires. Appendix A.3 indicates recent representative research wherein SD has been used in modeling sustainability in manufacturing and allied SCs. This has been attributed to two major reasons [138]. Firstly, the idea that sustainable development is conceived as being a “process” rather than a “project” whereby sustainability is not seen as a blueprint or a pre-conceived end state. Sustainability is a system state ideal and an ongoing process [139]. Secondly, sustainability entails that decisions and measures ought to be focused on the whole system

by sustaining harmony between its sub-systems and perception of cumulative impacts of actions. As sustainability is understood by assessing the state of environmental, social, and economic indicators while adequately addressing the interconnections between them. System dynamics as a paradigm bodes perfectly well to the aforementioned two conditions. As can be discerned from the “systemic” predisposition in of SD, its casts a wide net both “temporally” as well as “spatially”. The implication of which is that majority of research done in the SD framework is at the strategic level of operations. One may cite a number of works addressing the strategic aspects of sustainability in SCs. Carrying further the work of [140] on the social responsibility of SCs using SD and incorporating the product lifecycle and capacity planning [141], the SD model is used to model policy effectiveness to achieve optimal sustainability performance across the TBL.

Similarly, another study focused on strategic decision-making using SD looks at the modalities of policy-making in case of transition to sustainable manufacturing [142]. SD is used to model the effects of employee training, efficient equipment, and reduce costs and energy consumption as prerequisites to eco-invention. SD has also been used to assess organizational sustainability, [143]. The simulation is carried out at three levels, namely company level, SC level, and social level. Separate CLDs are constructed at the company and SC levels, showing the interrelationship between various KPIs. The study also invokes Maslow’s hierarchy of needs whence basic social needs and their areas of influence are categorized. Although SD finds its use primarily at the strategic level, but nonetheless, one may point to the studies where SD has been applied at the operational and tactical levels. Many players are often involved in SCs, which share information to coordinate material and product flows. As a result, SCs are complex systems with intrinsic dynamics, i.e., the performance of the system changes over time and is dependent on feedback loops [91]. SD models have been shown to assist decision-making in manufacturing SCs, including bullwhip effect, inventory management, reliability and risk management, etc. [144–147]. SD is used to model both forward and backward SCs. Given the importance of feedback loops in SD models, it is hardly surprising that reverse and closed-loop SCs account for a significant portion of SD models used in production and SC-related contexts. CE and closed loop SCs are fundamentally constituted by the feedback loops and this requirement is well addressed by the SD [91]. In order to better understand the application of the SD for assessing sustainability, various aspects of SD models have been lined up with their efficacy with regards to sustainability assessment in Table 4.

Table 4. Major aspects of the SD and their efficacy with regards to modeling sustainability.

Criteria	SD	Effects on Sustainability Assessment
Approach	Top-Down	Based on pre-defined model relationships in which the behavior of the system depends on the structure of the model. In sustainability modeling, pre-defined relationships amount to policies and thus is client friendly [129].
Object	Feedback	Objects in a system are flows (continuous quantity). SD is more appropriate for business thinking and physical processes [129]. Thus, reverse and closed-loop SCs constitute a lion’s share of SD models.
Space/Time	Continuous	Time is used as a variable such that the system may evolve over time. The sustainability assessment following the system is thus dynamic [129].
Feedback	Explicit	Uses closed-loop structures in which causal interactions and feedback effects are very important. Useful for understanding dynamics and feedback behaviors, in many social-ecological systems where sustainable pathways are sought [138].
Randomness	Deterministic	System characterized by differential equations such that the same input results in the same output all the time. The SD is used to project results to clientele [91].
Predictive power	Lower	Results take the form of simulations that enhance understanding of the structural source of behavior modes. Human agents as bounded rational policy implementers [93].

Table 4. Cont.

Criteria	SD	Effects on Sustainability Assessment
Abstraction level	Meso-Macro	The data magnification and strategic application imply that the units of modeling in case of SD are constituted at the organization level, e.g., modeling organizational sustainability in an SC organization [32].
Scope	Strategic	Owing to the systemic level, the SD is used to simulate long term sustainability, e.g., sustainable supplier selection in the auto industry [148].
Data	Qualitative	Data sources are broadly drawn. The data are subjective and largely judgmental, allowing for client-based sustainable policy-making. Less costly measurements required for different model variables with data for the quantitative modeling [94].
Use-case	Policy making/ causality	SD models owing to their systemic and policy nature find use in addition to individual researchers, international agencies, government agencies in case of sustainability, e.g., sustainable development of regional industries [149].

As described above, the SD finds its application along strategic and operational levels of operation. The description of which is given in Table A3. Among the articles collected, 26 deal with SD employed in sustainable manufacturing and SC exclusively, whereas in 15 articles, SD is used as a tool hybridized with other tools. The keyword network generated using Bibliometrix shown in Figure 15 shows three clusters.

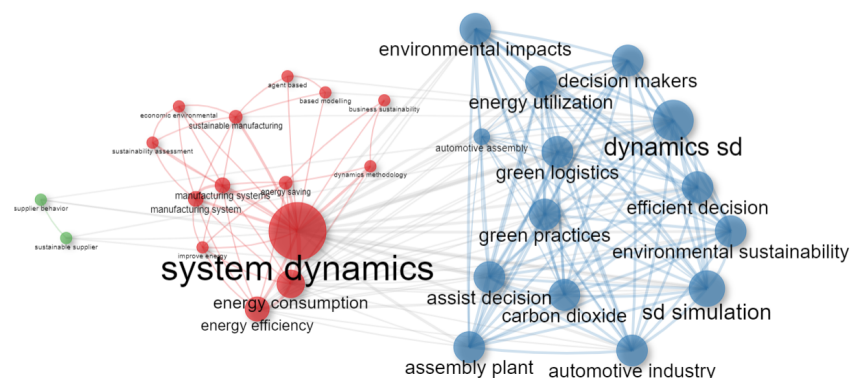


Figure 15. Keyword network of the collected research dealing with SD modeling in SC and manufacturing. The three clusters show predominance of keywords including green logistics, environmental impacts, automotive industry, and energy efficiency, respectively.

In the case of SD, a number of proprietary software is available and the most used among them is the VENSIM (which also has a free version called VENSIM PLE). Other commonly used proprietary software includes AnyLogic, Berkeley Madonna, GoldSim, iMODELLER, iTHINK, MapleSim, PowerSim studio, STELLA, and Wolfram SystemModeler. A number of platforms provide free modeling software, a detailed list of which is indicated in Appendix B.3.

4.4. Hybrid Simulations (HS)

Hybrid simulations (HS) find their beginning as early as the beginnings of simulation as a discipline, with attempts to bring together the continuous and discrete techniques [150]. HS is defined as combined use of two or more simulation models from the three main simulation approaches of DES, ABS, and SD. The classification of hybrid simulations based on discreteness and continuity has been conceived [151] along three categories, namely,

- Type 1 models: DES and SD hybrid models which contain both continuous and discrete elements;
- Type 2 models: ABS and DES hybrid models which contain either continuous and discrete elements;

- Type 3 models: ABS+DES+SD models which combine type 1 and type 2 models.

Although the use of HS proliferated during the 1960s and 1970s, this growth was curtailed owing to the lack of any computing support in form of any software. This all changed with the turn of the century when the OR problems became more and more complex and the growth of computing such as rise of AnyLogic software, HS modeling picked up pace. Unlike in the past, where the narrative was limited to continuous and discrete modeling, the HS modeling in the 21st century focused on the interaction between operational levels (modeled using DES and ABS) and strategic levels (modeled using SD). The use of ABS is invoked in situations where behavioral aspects are sought to be modeled [152]. The methodology of hybridization between the three models has been formalized using a number of frameworks.

A recent endeavor formalizes the hybridization of SD and DES through five major designs, namely, parallelism, sequential use, enrichment, interaction, and integration [75]. In the case of parallelism, the two modeling techniques are used in parallel, independently, such that both techniques working within the same boundaries, take an identical view of the situation. In the sequential approach, each model is used for a given purpose with very little overlap between the boundaries of the two. In the case of enrichment, one model (SD) forms the core of the technique while the other (DES) is used as an enhancement; both the models take the same view of the system with one being dominant throughout the process. In the interactive approach, the two models work independently but share the information with each other. This exchange takes place at a fixed time. In an integrated model, both the sub-models take the same view of the system while working within the same boundaries, the two are inseparable during the process such that the events in the DES are triggered by the threshold levels in the SD and, therefore, unlike the earlier methods, integrative techniques do not have set time gaps. Besides this, a few other frameworks that can be cited:

- Frameworks where all the three SD, ABS, and DES are addressed. The instances of which include generic 3M&S framework [129], system of system framework [153], and Multi-Paradigm simulation framework [154];
- Frameworks addressing DES and SD. Some characteristic frameworks include framework for hierarchical production [155], framework for manufacturing enterprise system [156], and framework in the healthcare domain [157];
- Frameworks addressing ABS and SD. Some of these include framework for SC [158] and framework using the complexity theory [159];
- Frameworks addressing DES and ABS. These frameworks can be instantiated in case of framework for determining output accuracy of models [160] and integration of ABS and DES frameworks [161].

The hybrid models exhibit different attributes and have been exploited differently in different studies. The attributes of the four types of hybrid simulations are tabulated in Table 5.

Modeling sustainability can be complicated and unpredictable, and it usually includes many layers of management decision-making, such as strategic and operational decision-making. This is especially true in the case of manufacturing SCs, which incorporate numerous subsystems and involves a variety of stakeholder groups. Developing models to react to such complexity demands knowledge of the features of sustainability and the system to be modeled, as well as a rethinking of the methodological components of M&S approaches that lend themselves to modeling of sustainable systems [162]. For effective sustainability modeling, a fit between approach, system, and problem is of fundamental importance. Prior to modeling and method/technique selection, a practitioner needs to consider the nature of the system and the problem at hand [163]. In contrast to the traditional techniques such as LCA, hybrid S&M techniques are far better in modeling CE but no single approach is able to appropriate all the aspects of CE. Traditional models lack the capability of sustainability metrics whereas industry ecology methods lack dynamic modeling capacities [4]. The combination of models gives the potential to simulate on

multiple scales which is a fundamental requirement in modeling sustainability. In the collected research works, sustainability has been modeled using hybrid methods. Table 6 indicates the hybrid methodology being employed in some of the recent research works in this context.

Table 5. Attributes of the four types of hybrid models.

Model	Attributes
DES-SD	It is a top-down approach while allowing for feedback, the approach permits for DES entities in modeling the system. Feedback loops capture links and time delays between the DES entities. Causality between the entities is ascertained while modeling dynamic and emergent behavior of the system. This hybrid is most researched in context of sustainability.
ABS-SD	SFDs are used to ascertain the states of the agents. ABS uses data from System dynamics to represent the heterogeneity of agents in a linked network. It may also employ feedback loop dynamics to govern agents' behavior as they progress from short to long term. It is the second most popular method in case of modeling sustainability.
ABS-DES	ABS encapsulates a high amount of flexibility and autonomy. It can simulate and capture DES entities' autonomous behaviors. Furthermore, using DES to represent events allows AB to give a great amount of flexibility in modeling varied agent behaviors, cognition, and decisions. DES outperforms ABS in terms of runtime performance, and it can track agent performance and construct specialized entities and events.
ABS-DES-SD	ABS uses self-organizing features to comprehend complicated adaptive systems. Emergent behaviors are simulated by ABS. DES takes into account resources, capabilities, and interaction rules to simulate different agents' behaviors using a series of events occurring at specified times in time. SD investigates the system's behavior patterns and interactions. Aggregate variables are used.

Table 6. Use of hybrid models in manufacturing and SC in the context of sustainability.

Model	Methodology
ABS-SD	Evaluation of industrial sustainability (IS) scenarios. IS is modeled as the interaction between policy (top-down) and resources(bottom-up). ABS is used to model the heterogeneity, behavior and interaction between the agents. SD models global variable behavior, system boundaries, and internal structure of agents [164].
	Sustainable Operations Management in Logistics. The model is applied to model safety, congestion, pollution, and quality of life. Deliverers' environmental conscious behavior is modeled using ABS and the SD is used to determine the impact of intelligent elements on system behavior [114].
DES-SD	Impact of electric vehicles on sustainability [165]. SD is used to model demand and power flows whereas DES analyzes control by modeling particular events.
	Integration the SD and DES for modeling the manufacturing enterprise system (MES) and SC in a hierarchical enterprise [166]. The hybrid model consists of SD model for MES and DES models for selected units which connect through SDDDES controller.
ABS-DES	Complex manufacturing system design [167]. The method uses a dynamic system of parallel multi-agent discrete events whereby ABS is used to simulate macro and micro levels with each sub-system being modeled as a dynamic DES structure.
	Sustainable product-service systems ABS is used to simulate the behavior of the customers and their relationship with the provider of PSS whereas the DES is used to simulate the provision process [168].

Table 6. *Cont.*

Model	Methodology
ABS-DES-SD	Hybrid model complementing LCA [169]. The SC is simulated using SD whereas ABS and DES are used to model market preferences. The DES is placed in the state chart of agent behaviors.
	Sustainable strategic management [170]. The model, simulated using AnyLogic, is constituted by four sub-systems such that financial resources and R&D technology are modeled using SD, the market sector using the ABS, and the operational sector including the SC is modeled using the ABS.

The HS models are executed through a number of software. The tools which allow for ease of linkages find greater use in HSs. Anylogic is the most used tool as it can model all the four modeling variations, namely, DES/ABS, SD/ABS, SD/DES and DES/ABS/SD models. Anylogic provides for the implementation of the depiction of common time and data exchange. Besides this, other software used in HS are Arena, Simul8, Flexim, Vensim, iTHINK, ExtendSim and NetLogo [150]. In addition to this, the studies also use bespoke solutions such as HLA-RTI, PoRTICo-RTI with JAVA augmentations, and other languages such as excel/VBA and VB.NET among others.

5. Discussion

The literature is rife with the application of the three simulation techniques in assessing the sustainability of manufacturing systems. This application, as can be gleaned from the preceding section, is nonetheless patchy at best. These limitations of application can be traced to the limitations of the aforementioned modeling techniques vis-a-vis CE. The literature points to a number of limitations of DES in modeling sustainability. Modeling using DES has been compared to “seeing trees for the forest” and such that it finds most of its use at operation level [162]. The consequence of which is that DES does not really cover the three aspects of the triple bottom line [171]. Another criticism leveled at DES is that it ignores the interconnections between high and low levels of the operations [172]. It is also reported that the DES does not allow for pro-active behavior which seriously curtails its efficacy in modeling social factors [173]. The limitations of applying the ABS for sustainability assessment are related to its complexity. The ABS model based on all the three aspects of sustainability is assessed to be extremely complex and too difficult to understand [174]. A similar criticism leveled at ABS is that such sustainability models, owing to high resolution, are very large [175]. As an implication of high resolution, the requirement of data is very large which in the case of sustainability assessment is either not present or in a form that may not be used as input to the ABS [174]. Along the same lines, the SD has been found to be lacking in sustainability assessment on many fronts. SD models have a tendency towards building systemic models with lesser concern for actual problem solving [176]. The implication of which is that the SD is more efficient in modeling outside the system rather than inside the system [173]. Similar to DES, SD also has issues with interconnections between the higher and lower level of operations such as SD fares poorly at operational levels. SD modeling has been found to be lacking in cases where interconnections between the TBL agents are sought in cases where there is no homogeneity [177]. An important observation with respect to all three models is that they are capable of running only one situation at a time. Even though they may be able to capture a wide range of variation in the evolving values of the variables, different parties or organizations with varying cultural or political objectives may bring different assumptions to the table and as a result see the situation differently image [171]. Elsewhere, the efficacy of the M&S frameworks has also been linked to the nature of the problem at hand, i.e., sustainability. The difficulty of balancing the triple bottom line is cited one of the barriers as the three factors may point to conflicting values [178]. Assessing sustainability is fundamentally a trans-disciplinary endeavor and, therefore, it has to be understood as a confluence of various disciplines such as engineering, ecology, law, politics

and sociology [179]. Finally, the data complexity and uncertainty render the optimum point as unstable affecting the success of the M&S frameworks [180].

Before any discussion on the potential future of M&S frameworks is occasioned, a discussion on the contemporary state of the industry is in order. The industry is presently undergoing a new revolution termed Industry 4.0 (I 4.0). Unlike the preceding Industry 3.0 paradigm where automation of individual machines and processes was sought, Industry 4.0 emphasizes on the digitization and integration of all the processes. To bring this about, Industry 4.0 is heavily reliant upon key technologies such as Virtual Reality (VR), Augmented Reality (AR), Artificial Intelligence (AI), and Digital Twins (DTs), among others, which are integrated through sensors, cloud computing, the Internet of Things (IoT) and, more importantly, real-time monitoring. The M&S frameworks are now increasingly being integrated with the I4.0 paradigm. The resultant framework is termed as Simulation 4.0 [17]. The primary constituents of this framework, as depicted in Figure 16, include in addition to the traditional simulation techniques, the concepts of digital twins (DTs), Augmented Reality (AR), Artificial Intelligence (AI), Petrinets Simulation (PS), Virtual Reality, and Virtual commissioning [181]. This integration between the two I4.0 and traditional M&S frameworks has been cited as beneficial for modeling sustainability [182]. The benefits cited are:

- I4.0 enables modelers with analyzing and representation of the system at both low and high-level resolution;
- Possibility to automate the modifications like what-if questions;
- Modelers have greater power with regards to understanding and analysis of the integration of the TBL measurable factors within the system.

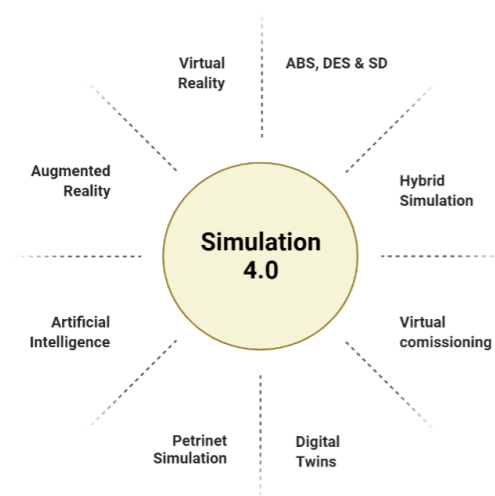


Figure 16. Simulation 4.0—Simulation approaches applied to industry 4.0.

Despite the benefits of the I4.0 for modeling sustainability, it has been argued that the M&S framework requires a major overhaul [182]. Although the I4.0 framework has provided with greater data transparency, computation power, and speed, the greater objectives of CE are far from being realized. The literature points out the following weaknesses in the current M&S framework.

- Current frameworks are deeply invested in the states of equilibrium and optimality. A complex system that engenders the TBL needs not necessarily have a unique optimal state [180];
- Current frameworks are designed while assuming industrial systems and SCs are closed systems rather than open systems. There is an implicit assumption that these systems can only exhibit function and not evolution and, as a result, any structural change in the system renders the models useless [183];

- It has also been argued that the sciences that deal with sustainability are fundamentally different than those that give rise to sustainability issues while the former are engaged with the “causes”, the latter are engaged with the “symptoms”.

In view of the preceding discussion, it is evident that there is a manifest gap between the current state of M&S methodology and the requirements of modeling a circular economy. It is inevitable that a new paradigm of M&S frameworks is brought about. The prerequisites of such a framework can be delineated as:

- Utilizing the benefits of hybrid M&S techniques which have greater efficacy in the assessment of complex systems;
- Integration of the traditional M&S techniques with the I4.0 paradigm whereby models may have greater granularity and abstraction;
- Sustainability systems are open and complex systems that warrant constantly changing processes where the optimum point is not known in advance.

6. Conclusions

This article has sought to exhaustively cover various aspects of M&S in the context of sustainability but nonetheless, various aspects of M&S have not been addressed, including the sustainability metrics, automating technologies such as AR, VR, IIoT, DTs in modeling, and actual data requirements of given modeling techniques. However, in the limited space of a research article, one can only touch upon a few themes. This article has not delved into the mathematical techniques such as Monte Carlo simulation, Mixed-integer linear programming (MILP), nonlinear programming, space mapping, etc., but is limited to DES, ABS, and SD and their hybrids. The reason for the same is that mathematical methods invoke to a greater degree the concept of optimization which in itself is a vast topic and could not possibly have been tackled by this article. As discussed above, modeling of sustainability in the case of manufacturing and SCs requires tools that are capable of multi-level granularity and magnification such that both technical and meta-technical aspects of SCs are taken into consideration. Owing to the pre-eminence of DES in modeling, an overwhelming amount of research has been carried out in either energy modeling or flow modeling. A consequence of this is that it has limited the scope of M&S to the short-term operational levels. The DES has had a head start among the three techniques but in case of CE, ABS and SD have seen greater success in the recent past. The trend of increased use of ABS has also been alluded to elsewhere [8]. Apart from having a systemic/macro view that bodes well with sustainability analysis, there has been increased recognition and software availability in the case of ABS. This may also be attributed to a positive feedback effect wherein an increase in the number of studies results in further increase in the number of new studies undertaken. A substantial amount of research, specifically in recent times, has addressed hybrid simulations. Hybrid models allow for multiple viewpoints in a single endeavor, thereby attenuating the issues which are faced in the individual methods. Hybrid models find prolific application in research but there is a dearth of review work on them. Additionally, exclusive software support for the hybrid methods is also lacking. Published research also points out to hybrids of DES, ABS, and, SD with Industry 4.0 technologies with some instances, including DES and ABS with DTs [184], DT and CPS [185], SD and CPS [186], among others. However, research in this context within the CE framework is scarce. M&S frameworks present an exciting setting whereby the CE could appropriately and objectively be brought about in manufacturing and allied SCs. The application of M&S techniques is diverse on the account of the multitudes of techniques and their application. Nonetheless, their application suffers from myopic implementation. The limitations may be ameliorated by a new framework that eschews closed-system, incorporates the I4.0 framework, and utilizes the benefits of the hybrid simulation techniques.

Finally, the intended evolution from Society 4.0 to Society 5.0 is not just an evolution of technical expertise but that of a whole paradigm wherein a holistic and nature-positive science must be the basis of change. Similarly, when one points to a novel simulation paradigm, it does not just incorporate more precise and accurate modeling but a modeling

that is itself dynamic and open to changes. Such a framework may well have to move away from a calculus-based Newtonian deterministic framework to a more holistic understanding of human–nature synergy while taking into account the various aspects indicated above.

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Appendix A. Application M&S Frameworks in the Industry in Context of CE

In this section, some of the recent applications of Discrete Event Simulation (DES), Agent-Based Simulation (ABS), and System Dynamics (SD) are indicated. The research work indicated is a sub-set of the compiled papers and as such is composed as being representative of the state of contemporary research in the field.

Appendix A.1. Application of DES in the Industry

The table indicates some of the aspects of manufacturing and SCs that have been simulated within the framework of sustainability using DES in the recent past. Although majority of the studies undertaken using the DES can be situated on the operational and the tactical level, nonetheless, some of the studies addressing the strategical issues have also been included.

Table A1. Application of DES in modeling sustainability in manufacturing and allied SCs.

Theme	Methodology	Level
Sustainability Cockpit [68]	Resource optimization by measuring material, machine and energy utilization. Anylogic used as the simulation tool. Bill of material (BoM) from the ERP is used to ascertain material usage	Tactical-Operational
Sustainable facility design [187]	Using genetic algorithm with DES. Environmental sustainability is described in terms of energy utilization which itself is assumed to be contingent on machine utilization. Social sustainability is modeled using work shifts	Strategical
Information-based resource allocation [188]	Forest SCs, which exhibit stochastic-dynamic behavior, are studied with queuing at center of focus. The criteria of trucking distance, storage volume, and moisture content are simulated using seven scenarios using Witness DES software	Strategical-Tactical
Eco-efficiency of production systems [189]	DES used to simulate the lifecycle of the products by integrating Ecoinvent-LCI database. Identifying the potential areas of improvement the processes are expressed as environmental value stream mapping (EVSM). DES is carried out using PlantSimulation software	Operational
Sustainable additive and subtractive manufacturing [190]	Production lines in context of TBL by comparing subtractive and additive manufacturing. DES is used in a dynamic setting with changing order volumes and types	Tactical

Table A1. *Cont.*

Theme	Methodology	Level
Product life cycle simulation [90]	Based on appropriating the resource flows using Lifecycle simulation (LCS) based on DES. LCS used to trace resources from sources to the end of life, environmentally and economically. Formulating a complex system of interactions between resources called as System of Systems (SoS)	Strategical
Resource sharing in sustainable production [92]	Different scenarios in sourcing of resources in a garment factory are simulated using DES. The resource sharing in case of mass customization is assessed	Strategical-Tactical
Simulating emissions in freight [191]	The behavior of common scenarios of transport operations in the SC, including greenhouse gas emissions and travel time of operating routes investigated	Operational
Energy resource management [89]	Modeling the sourcing energy from third party suppliers and minimizing the carbon emission. The instantaneous need of energy which is stochastic is modeled	Operational
Simulating overall equipment efficiency (OEE) [98]	The DES is used to simulate the energy OEE of the discrete manufacturing facilities. The data from a CNC machine are used to evaluate the model	Tactical-Operational
Integrating human factors using DES [97]	Modeling patterns of human fatigue and recovery in industrial contexts. Simulation based on DES designs a production system that is more productive while also mitigating the operational hazards	Operational-Tactical

Appendix A.2. Application of ABS in the Industry

The table indicates some of the aspects of manufacturing and SCs that have been simulated within the framework of sustainability using ABS in the recent past.

Table A2. Application of ABS in modeling sustainability in manufacturing and allied SCs.

Theme	Methodology	Level
Supplier risk mitigation [128]	ABS conducted using NetLogo wherein the decisions with regards to sustainable suppliers by the SC managers who are interviewed using vignettes	Strategic
Resource sharing in freight transport [134]	Using NetLogo software the empty transportation is sought to be reduced. Trucks and hubs are modeled as agents	Tactical-Operational
Simulating the horizontal co-operation in logistics [126]	Simulating the carbon dioxide emissions in case of cooperation between logistics departments using Anylogic 8.0 software	Strategical-Tactical
Sustainable supplier selection [192]	A multi agent system (MAS) used for sustainable order allocation and supplier selection. Suppliers are evaluated using Fuzzy Inference system (FIS) using GAMS inside the JADE environment	Strategic-Tactical
Modeling industrial symbiosis [193]	Simulating the use of waste from one industry to another. The model uses enterprise input output model (EIO) with the ABS. ABS is used to simulate the cost sharing in case of collaboration	Tactical
Resilience and ripple effect in SCS [194]	Impact of blockchain technology is assessed on the resilience of SCs. Assuming two scenarios, one in absence of BCT and another vice versa, uses run time, disruption, varying input, and number of runs as the input	Strategical
Resource sharing [134]	The multi agent model simulates the trucks in a freight network operating across Canadian cities on the NetLogo software. The KPIs included are cost indicators, social indicators, and environmental indicators	Operational
Efficiency in resource investment [123]	Using the modified EURACE agent based framework by coupling environmental and macroeconomic dimensions. Simulation is used to explore the policies for investment in resource efficiency	Strategic
Real time energy modeling [127]	Using the data from the industrial robots which is analyzed using an agent-based framework while the optimization problem is carried out using IBM ILOG OPL. Data acquisition is using Arduino ATmega 328 electronics platform	Operational

Table A2. *Cont.*

Theme	Methodology	Level
Sustainable manufacturing system (SMS) [195]	Using Anylogic, model a configuration of SMS by taking into account the minimization of the total cost, total energy consumption, and CO ₂ emissions. Variables used are supplier, factory, and warehouse	Operational-Tactical
Energy-Efficient Scheduling [37]	Scheduling of manufacturing systems through collaboration between cyber-physical production and energy systems. A multi-agent architecture elaborating predictive and reactive energy-efficient scheduling using JADE framework	Operational

Appendix A.3. Application of SD in the Industry

The table indicates some of the aspects of manufacturing and SCs that have been simulated within the framework of sustainability using SD in the recent past.

Table A3. Application of SD in modeling sustainability in manufacturing and allied SCs.

Theme	Methodology	Level
Social sustainability through SD [141]	SD in Reverse Logistics Social Responsibility (RLSR). The model takes into account interrelated sustainability dimensions adopting a product lifecycle approach with uncertainties	Strategic
Recycling in a closed-loop SC [196]	Using VENSIM PLE software to optimize the recycling and collection of waste material in an electrical factory	Tactical
Modeling eco-innovation processes in manufacturing firms [142]	Using VENSIM software to model variables, including financial, raw material, equipment, production, and personnel and drawing up the difference between eco-variables and traditional variables	Strategic
Sustainability assessment in make-to-order (MTO) SCs [197]	MTO SCs, typical in aerospace sector, highly complex situations are modeled using a hybrid modeling tool of SD, ABD, and DES leveraged by MCDA using Anylogic software	Strategic-Operational
Business cases for ecodesign implementation [198]	Using Ecodesign Maturity Model (EcoM2), through meta-analysis, SD is used for modeling organizational capability in the product development space	Strategic
Model for Organizational Sustainability [143]	Holistic approach as how organizations interact with environment both internally and externally. Using SD and Viable System and modeling levels of company, supply chain, and society measures on VENSIM	Strategic
Policy-making for CO ₂ mitigation [199]	Energy modeling in cement industries using energy efficiency measures. Using VENSIM PLE software, study carries out modeling at three levels, namely government, society, and manufacturers	Strategic
Sustainable supplier selection in automotive industry [148]	Data from expert interviews used, simulated using SD in fuzzy environment in VENSIM to find the best potential sustainable supplier	Strategic
Effect of rapid prototyping implementation on SC sustainability [200]	A generic SD model simulating the RP-adapted SC. Using VENSIM software and modeling economic, social and environmental KPIs	Tactical
Sustainable supplier management [201]	A virtual warehouse simulated using VENSIM. Conceives two models one with and other without inventory sharing system	Tactical

Appendix B. Open-Source Software Used in M&S Frameworks

Through the years, a number of M&S tools have been developed each with a specific objective. Each approach indicates a specific programming syntax with differences in the generality, usability, modifiability, scalability, and performance. The landscape of S&M software is thus populated diversely, a diversity including both open-source and proprietary solutions. This section provides details and use-cases of some of the open-source software in the three simulation frameworks.

Appendix B.1. Open-Source DES Software

The software development in case of DES is the earliest with the development of SIMSCRIPT in 1962. Since then, numerous generic and context specific tools have been developed. A detailed evolution of these tools have been presented in [202]. Table A4 indicates some of the commonly used open-source DES software and their sustainability specific use-cases.

Table A4. Open-source DES software in use in the industry. Other free software include CPN Tools, Fascimile, SIM.JS, SystemC, and Simula.

Software	Description	Use-Case
OMNet++	C++-based modular, component library and framework used in network simulators	Comparison of simulation tools [203] Vehicle rerouting [204] Industrial control systems [205]
NS-3.35	A DES simulator for internet systems primarily used in education and research licensed under the GNU GPLv2 license	Vehicle routing [206] Vehicular Ad Hoc Networks [207]
SimPy 4.02	A DES process-based framework based on python used to model components such as customers, vehicles, and agents	Inventory optimization [208] sustainable physical internet-integrated SCs [209] smart manufacturing [210]
JaamSim	DES program with a drag-and-drop user interface, interactive 3D visuals, input and output processing, and model construction tools and editors	Inventory management [211] sustainable multicomponent-distributed manufacturing [212] lean manufacturing [213]
DESMO-J	Stands for Discrete-Event Simulation and MOdelling in Java. The software provides java classes for stochastic distributions, static components, scheduling, and reporting	Performance analysis of assembly lines [214], cost analytics [215], production design [216], worker performance [217], optimal stock levels [218]
URURAU	Multi-platform program that enables users to create models using a graphical interface or directly in source code. Used as a learning tool as well as a tool for modeling and simulation of discrete systems	Energy modelling in manufacturing [219], green logistics [220], carbon monoxide emission [221], logistics emissions [191]
Ptolemy II	Used in concurrent, real-time, embedded systems. Characterized by use of well-defined computation models that regulate the interaction between components.	Renewable resource sourcing [222], industry 4.0 production line [223], cyber-physical system [224],
PowerDEVS	A generic DEVS modeling and simulation addressing hybrid system simulation. The environment enables the creation of increasingly sophisticated systems by specifying atomic DEVS models in the C++ language, which can then be visually connected in hierarchical block diagrams	Cyber physical systems [225], energy modeling [226]
Salabim	An object-oriented DES open-source python based library. It uses the process description technique in the likeness of Simula. DES, queue handling, resources, statistical sampling, and monitoring are all included in the program	Throughput time in manufacturing [227], manufacturing scheduling [228], process planning, and dynamic scheduling [229],

Appendix B.2. ABS Software

The development of software tools for ABS has seen most growth in the last few years. Research points to large number of such tools [121]. Table A5 indicates some of the most commonly used tools and their sustainability specific use-cases.

Table A5. Open-source ABS software in use in the industry. Other free software include Adaptive Modeler, Cougaar, and StarLogo.

Software	Description	Use-Case
AgentScript	Inspired by the Netlogo, is a javascript library, lets the programmer model with three ingredients	Agent-based Machine learning in factory automation [230], Integration and testing for MA engineering [231]

Table A5. Cont.

Software	Description	Use-Case
Ascape	Tool for developing general and multipurpose simulations written in java where agents are implemented as JAVA classes	Simulating human factor in production [232], using grounded theory for simulating organizational behavior in a plastic factory [233]
Brahms	JAVA-based agent/object-based belief-desire-intention (BDI) language. The Brahms and JAVA agents interact with each other	Organizational behavior [234], Verification of Human–Robot Teamwork [235]
Flame	Flexible Large Scale Agent Modeling environment (FLAME) is a general purpose simulation tool. Agents are construed as objects having states, functions, and set pf variables	Comparison of various ABS frameworks for aerial transportation [236]
GAMA	Simulating 2D and 3D spatially explicit ABS using GAML modeling language. Extensive libraries for agent architecture designing and spatial analysis functions	Material flows in SC [237]
HLA_Agent	A C++-based tool for the distributed simulation of ABS, which combines the sim_agent agent toolkit and the High Level Architecture (HLA), finds major use in manufacturing and SC.	Distributed manufacturing [238], Distributed SC [239], green transportation [240]
NetLogo	It is a multi-agent programmable modeling environment in NetLogo language and is fully inter-operable in JAVA and other JVM codes	Sustainable SC [241], Routing in flexible manufacturing [242], short cycle SC [243]

Appendix B.3. SD Software

Table A6. Open-source SD software in use in the industry. Besides this, some other software include Sphinx SD Tools, MapSim and StochSD.

Software	Description	Use-Case
Insight maker	A javascript and browser-based SD modeling tool, has extensive System Dynamics support including powerful support for dimensional analysis and unit conversion	Solid waste management [244], profitability of automation [245]
NetLogo	Agent-based simulation tool that also supports SD modeling	Dynamical systems [246], Multi-Agent Collaborative Planning in SCs [247], waste and cost reduction in lean manufacturing [248], Transportation Modeling [249]
Open Modelica	Maintained by Open-Source Modelica Consortium (OSMC) in collaboration with Linköping University and written in C++, used in academic and industrial environments	Building Digital Twins of Sustainable Cyber-Physical Systems [250], additive manufacturing [251], energy modeling of industrial robots [252]
Simantics System Dynamics	Large hierarchical models with multidimensional variables are simulated using this tool. Traditional stock and flow diagrams and causal loop diagrams are used to generate the models. Different visual tools are provided to assess simulation results and model structure	Verification of industrial process control systems [253], automatic generation of LCA [254]

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